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Combinatorial trees arising in the study of interval exchange transformations

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ABSTRACT

In this paper we study a new class of combinatorial objects that we call *trees of relations* equipped with an operation that we call *induction*. These trees were first introduced in Ferenczi and Zamboni (2010) [3] in the context of interval exchange transformations but they may be studied independently from a purely combinatorial point of view. They possess a variety of interesting combinatorial properties and have already been linked to a number of different areas including ergodic theory and number theory—see Ferenczi and Zamboni (2010, in press) [3,4]. In a recent sequel to this paper, Marsh and Schroll have established interesting connections to the theory of cluster algebras and polygonal triangulations: Marsh and Schroll (2010) [5]. For each tree of relations G, we let $\Gamma(G)$ denote the smallest set of trees of relations containing G and invariant under induction. The induction mapping allows us to endow $\Gamma(G)$ with the structure of a connected directed graph, which we call the graph of graphs. We investigate the structure of $\Gamma(G)$ and define a circular order based on the tree structure which turns out to be a complete invariant for the induction mapping. This gives a complete characterization of $\Gamma(G)$ which allows us to compute its cardinality in terms of Catalan numbers. We show that the circular order also defines an abstract secondary structure similar to one occurring in genetics in the study of RNA.

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1. Introduction

In [3] we introduced a new induction algorithm for a family of interval exchange transformations T in the hyperelliptic Rauzy class. This algorithm, called the *self-dual induction*, provides new insight into the symbolic dynamics of the trajectories [4]. Our aim was to describe completely the trajectories of points, and to relate both the combinatorial and dynamical properties of the underlying system to the number-theoretic properties of an associated multi-dimensional continued fraction algorithm. If T is an exchange on k intervals, then at each stage of our induction, we induce T (by first return) on a disjoint union of $k-1$ sub-intervals E_j, each containing the point β_j of discontinuity of T^{-1} and whose endpoints are in the orbits of the discontinuities of T. This process defines a multi-dimensional continued fraction algorithm generated by the $2k-2$ parameters $\{l_j, r_j\}_{1\leq j\leq k-1}$ where l_j is the distance from β_j to the left endpoint of E_j and r_j the distance from β_j to the right endpoint of E_j.

As soon as $k \geq 3$, the $2k-2$ parameters $\{l_j, r_j\}_{1\leq j\leq k-1}$ are not independent and in fact satisfy $k-2$ symmetric relations of the form $l_i = l_j$, or $r_i = r_j$ or $l_i + r_i = l_j + r_j$ for some $i \neq j$. At each state of the induction, these relations, which are a consequence of the isometry of the transformation T and the nature of the underlying permutation, may be coded by a tree on $k-1$ nodes (labeled 1 through $k-1$) with labeled edges, where the labels take on three possible values corresponding to the three different kinds of relations. Thus a labeled edge in the tree between nodes i and j indicates a relation between parameter $x \in \{l_i, r_i\}$ and $y \in \{l_j, r_j\}$, and the exact form of the relation is given by the edge label. These trees, which we call *trees of relations*, are at the very core of the dynamics of hyperelliptic interval exchange transformations, and in fact in [3] we show that the entire combinatorial description of the trajectories of T may be deduced directly from them.

In the present paper we define and study trees of relations, equipped with the operation of induction, from a purely combinatorial view, that is removed from the context of interval exchange transformations. Very simply, a tree of relations is a tree in which each edge is labeled by $+$, $=$, or $-$, and such that no two adjacent edges have the same label. Fig. 1 depicts an example of a tree of relations with ten vertices. These trees, equipped with the operation of induction, constitute a new discrete structure possessing rich combinatorial properties. Together they define directed graphs whose vertices consist of trees of relations with vertices 1 through $k-1$, and where the directed edges between vertices are given by the induction mapping.

An outline of the paper is as follows. In Section 2 we consider an example of an interval exchange T on 4-intervals, to illustrate the induction algorithm in the context of interval exchanges.

In Section 3 we define and study the basic properties of trees of relations. We define the induction mapping in purely combinatorial terms as a mapping from trees of relations to trees of relations.

In Section 4 we show that for every tree of relations G, the set $\Gamma(G)$, defined as the smallest set of trees of relations containing G and invariant under induction, may be endowed with the structure of a connected directed graph. We call the directed graph $\Gamma(G)$ the graph of graphs of G.

In Sections 5–7, we investigate the structure of the graph of graphs $\Gamma(G)$. For this purpose we introduce in Section 5 two auxiliary notions: *shapes* and *fillings*. A shape is a tree of relations in which the vertices are unlabeled—they represent the skeleton of the tree, while the filling represents the passage from shapes to trees. We then show that the trees in $\Gamma(G)$ realize every possible shape.

In Section 6 we define a circular order on the vertices of a tree of relations which is determined by its tree structure. We show that two fillings of a shape are in the same $\Gamma(G)$ if and only if they define the same circular order on their respective vertices: the circular order is a complete invariant for the induction mapping, and thus gives a full characterization of $\Gamma(G)$.

In Section 7 we use this invariant to count both the number of shapes and the cardinality of $\Gamma(G)$, using formulas involving Catalan numbers.

In Section 8 we discuss an interesting connection between the circular structure defined in Section 6 and a similar structure occurring in genetics in the study of RNA.

Recently, Marsh and Schroll have written a sequel to this paper, further extending the combinatorial theory developed herein and establishing interesting and surprising connections to polygonal m-angulations, Fuss–Catalan combinatorics, and the theory of cluster algebras (see [5]).

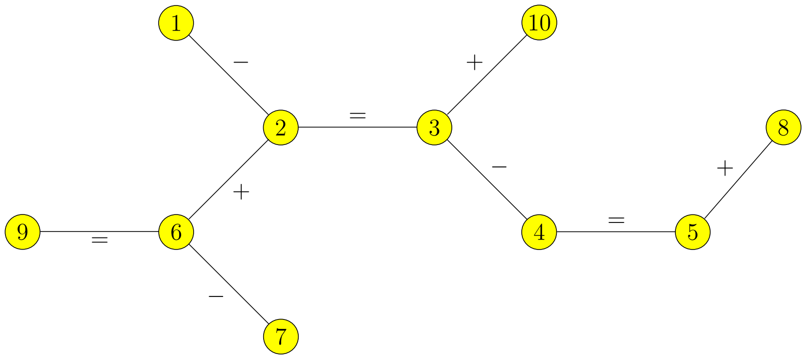

Fig. 1. A tree of relations on 10 vertices.

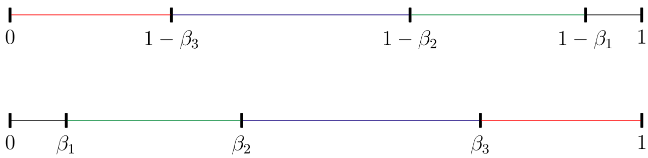

Fig. 2. A symmetric 4-interval exchange transformation.

2. Interval exchange transformations

Let us consider the interval exchange transformation T on 4-intervals as shown in Fig. 2 (by convention, all intervals are open on the right, closed on the left). The transformation T maps by isometry the first interval $[0, 1-\beta_3[$ onto the interval $[\beta_3, 1[$, the second interval $[1-\beta_3, 1-\beta_2[$ onto $[\beta_2, \beta_3[$, the third interval $[1-\beta_2, 1-\beta_1[$ onto $[\beta_1, \beta_2[$, and the fourth interval $[1-\beta_1, 1[$ onto $[0, \beta_1[$.

For convenience, we further impose the initial condition

$$0 < \beta_1 < 1-\beta_3 < \beta_2 < 1-\beta_2 < \beta_3 < 1-\beta_1$$

so β_1 is in the interval $E_1 = [0, 1-\beta_3[$, β_2 in the interval $E_2 = [1-\beta_3, 1-\beta_2[$, and β_3 in the interval $E_3 = [1-\beta_2, 1-\beta_1[$. For each $j \in \{1, 2, 3\}$ we consider the two parameters l_j, r_j where l_j and r_j are defined as the respective distances between the point β_j and the left and right endpoints of E_j; thus $|E_j| = l_j + r_j$ is the length of E_j.

We remark that there are two relations between these parameters, namely that $r_1 = r_3$ and $l_2 = l_3$; they are a consequence of the underlying isometry of T and the choice of the permutation by which we rearrange the intervals. We record (or code) them as follows: for $r_1 = r_3$ we write $1\hat{-}3$ (or equivalently $3\hat{-}1$) and for $l_2 = l_3$ we write $3\hat{+}2$ (or equivalently $2\hat{+}3$). We may combine these two expressions by forming a tree with vertices $\{1, 2, 3\}$ and with an undirected edge labeled $-$ between 1 and 3 and one labeled $+$ between 2 and 3 as shown in Fig. 3; this tree is denoted also by $1\hat{-}3\hat{+}2$ or $2\hat{+}3\hat{-}1$ (see the beginning of Section 3).

The self-dual induction defined in [3] starts from the three intervals $E_{1,0} = E_1, E_{2,0} = E_2, E_{3,0} = E_3$, and creates three smaller intervals $E_{1,1}, E_{2,1}, E_{3,1}$ (thus they are no longer adjacent). By iteration, we obtain three families of nested intervals $E_{1,n}, E_{2,n}, E_{3,n}$. At each step of the induction we consider the sub-interval $E_{i,n}$ containing the special point β_i, and recalculate the corresponding parameters l_i, r_i. It turns out that at each stage there will be two relations between the parameters of the following form: for some $i \neq j$, $l_i = l_j$, which we code by $i\hat{+}j$ or equivalently by $j\hat{+}i$, or $r_i = r_j$, which we code by $i\hat{-}j$ or equivalently by $j\hat{-}i$, or $|E_i| = |E_j|$, or equivalently $l_i + r_i = l_j + r_j$, which we code by $i\hat{=}j$ or equivalently by $j\hat{=}i$.

The complete definition of the self-dual induction was made in [3]; as it is not necessary to the understanding of the present paper, we choose to follow first what happens on one example and

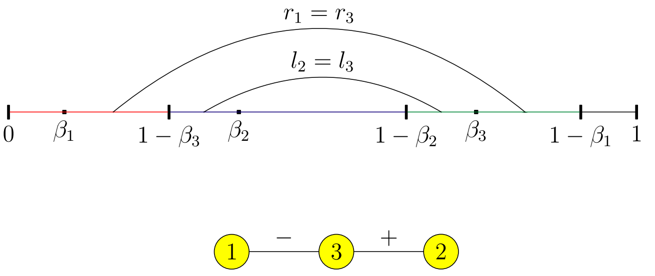

Fig. 3. The coding of the parameters in state 0.

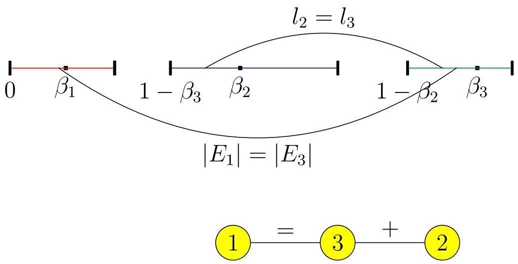

Fig. 4. The coding of the parameters in state 1.

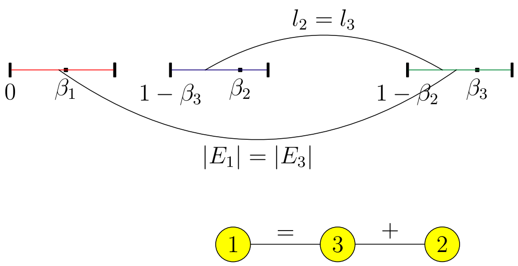

Fig. 5. The coding of the parameters in state 2.

postpone the full definition to Section 3 below, as it requires the full definition of the induction operation on trees in Section 2 below. Thus, suppose that in state 0 (the initial state) we have $r_1 > l_1$, $r_2 > l_2, r_3 > l_3$. Then, in passing to the subsequent state (state 1), each interval E_i is cut from the right by the amount l_i, as shown in Fig. 4. It follows from the previous relations that the new parameters satisfy the new relations $l_2 = l_3$ (or $2\hat{+}3$) and $|E_1| = |E_3|$ (or $1\hat{=}3$).

Suppose that in state 1, the corresponding parameters satisfy $l_1 > r_3, r_2 > l_2, l_3 > r_1$ (this happens whenever the parameters in state 0 satisfy $l_1 + l_3 > r_1 = r_3 > \max(l_1, l_3)$ and $r_2 > 2l_2$, which can be realized). Then the interval E_2 is cut from the right by the amount l_2, while the other intervals are not cut. Although the new parameter values of l_2 and r_2 differ from the corresponding values in the previous state, these two parameters were not involved in the preceding relations and hence the coding remains unchanged as shown in Fig. 5.

Suppose that in state 2 the corresponding parameters satisfy $l_1 > r_3, l_2 > r_2, l_3 > r_1$ (again there are initial values of the parameters for which this happens). To go to state 3, the interval E_1 is cut from the left by the amount r_3, and E_3 is cut from the left by r_1, while E_2 is cut from the left by r_2. This gives rise to the coding $3\hat{+}1\hat{=}2$ as shown in Fig. 6.

Suppose that in state 3 the corresponding parameters satisfy $l_1 < r_2, l_2 < r_1, l_3 < r_3$. In passing from Fig. 6 to Fig. 7 the interval E_1 is cut from the right by the amount l_2 and E_2 is cut from the right by l_1, while E_3 is cut from the right by l_3.

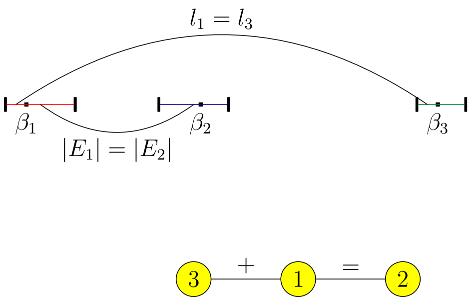

Fig. 6. The coding of the parameters in state 3.

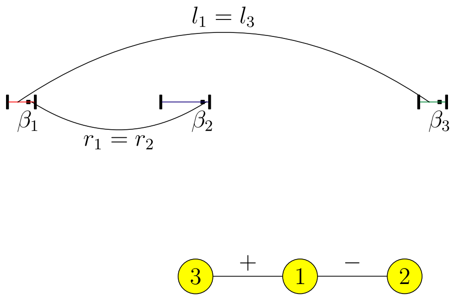

Fig. 7. The coding of the parameters in state 4.

As it turns out, each state has been coded by a tree of relations. We next build a graph whose vertices consist of all trees of relations coding the possible states, and where there is a labeled directed edge between any two adjacent (or consecutive) states. The edges are labeled by either $+$, if the intervals are cut from the left, or $-$, if they are cut from the right. The resulting graph is shown in Fig. 17 below, where the highlighted edges represent the initial path between consecutive states outlined in the present example. If we iterate the self-dual induction infinitely many times we obtain an infinite path in this graph.

3. Trees of relations and induction

By a *tree* we mean a non-oriented connected graph which has no cycles.

Definition 3.1. A tree of relations on a finite nonempty set K is a tree G satisfying the following three conditions:

- The vertices of G are the elements of K.
- Each edge of G is labeled with $\{+, =, -\}$.
- No two adjacent edges of G have the same label.

Notation. Throughout this paper, we consider edges labeled with $\{+, =, -\}$. *We use the notation* $a\hat{+}b$ *(resp.* $a\hat{=}b$, $a\hat{-}b$*) to denote the edge labeled* $+$ *(resp.* $=$, $-$*) between the vertices a and b*. By further abbreviation, in describing a given tree of relations G we write just (for example) that $a\hat{+}b$ in G to express that there is an edge $a\hat{+}b$ in G, and $a\hat{+}b\hat{=}c$ instead of $a\hat{+}b$ and $b\hat{=}c$. The hats are used only to avoid writing expressions like $1 = 2$ or $1-2 = 3$, and thus are not needed in pictures or in expressions like a $+$ edge. Clearly $a\hat{+}b$ is equivalent to $b\hat{+}a$, and the same if we replace $+$ by $-$ or $=$.

Example 3.2. The tree given in Fig. 1 can be described in many equivalent ways, for example by $1\hat{-}2\hat{=}3\hat{+}10$, $2\hat{+}6\hat{=}9$, $6\hat{-}7$, $3\hat{-}4\hat{=}5\hat{+}8$, or alternatively $8\hat{+}5\hat{=}4\hat{-}3\hat{=}2\hat{+}6\hat{-}7$, $6\hat{=}9$, $2\hat{-}1$, $10\hat{+}3$.

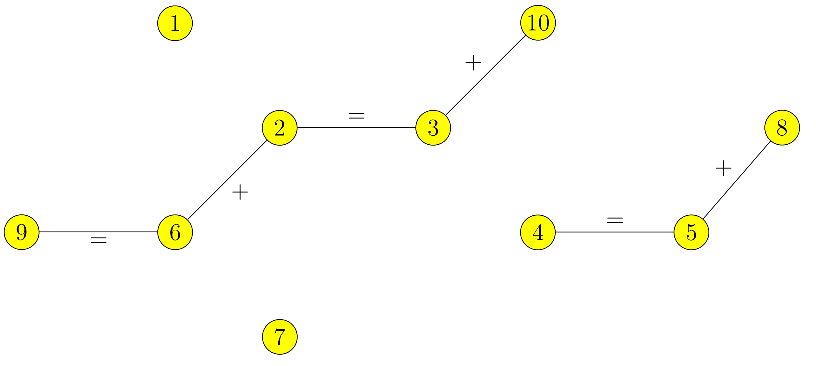

Fig. 8. The positive chains in Fig. 1.

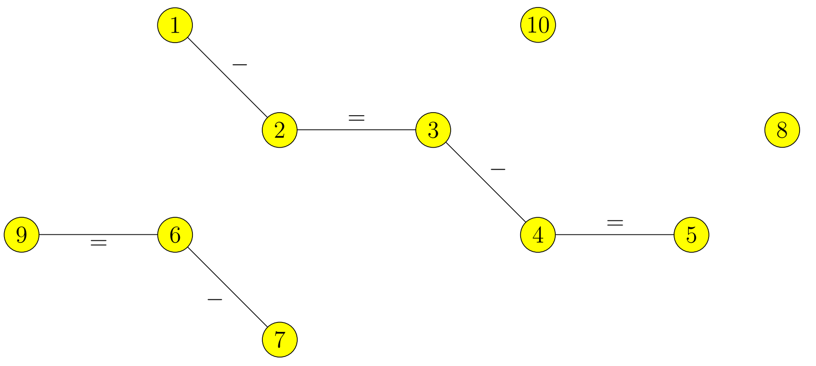

Fig. 9. The negative chains in Fig. 1.

With each tree of relations G on K we associate three bijections $s, t, u : K \to K$ defined as follows: for each $a \in K$ we put:

- $s(a) = b$ if $a \hat{=} b$ for some $b \neq a$. Otherwise set $s(a) = a$.
- $t(a) = b$ if $a \hat{+} b$ for some $b \neq a$. Otherwise set $t(a) = a$.
- $u(a) = b$ if $a \hat{-} b$ for some $b \neq a$. Otherwise set $u(a) = a$.

It is immediate that

$$s^2 = t^2 = u^2 = Id.$$

Definition 3.3. Let G be a tree of relations. By a positive chain we mean a maximal connected subtree of G having no $-$ edges. Similarly a negative chain is a maximal connected subtree of G having no $+$ edges. By a signed chain we mean either a positive or a negative chain.

Figs. 8 and 9 illustrate the positive and negative chains respectively of the tree of relations given in Fig. 1.

We next define an operation on trees of relations which we call *induction*. This operation associates with each tree of relations G on K and each signed chain B of G a tree of relations $J_B(G)$ on K as follows:

Definition 3.4. Let G be a tree of relations on K, with first bijection s, and B be a signed chain. The tree of relations $J_B(G)$ is defined by the vertices a, $a \in K$, and the following edges:

- if $a \in B$, $b \in B$, and $a \hat{+} b$ in G, then $s(a) \hat{=} s(b)$ in $J_B(G)$,
- if $a \in B$, $b \in B$, and $a \hat{-} b$ in G, then $s(a) \hat{=} s(b)$ in $J_B(G)$,

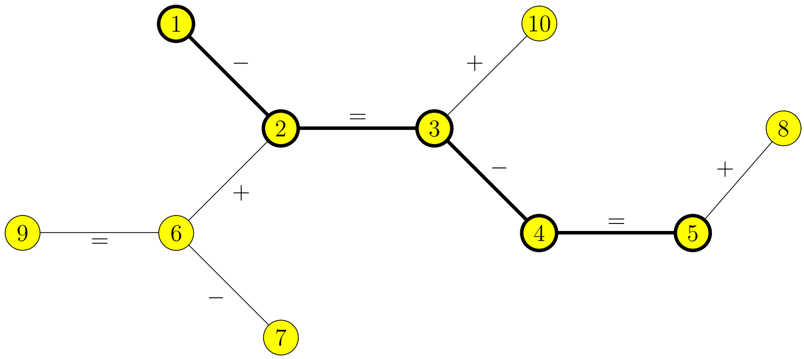

Fig. 10. An induction on the tree of Fig. 1.

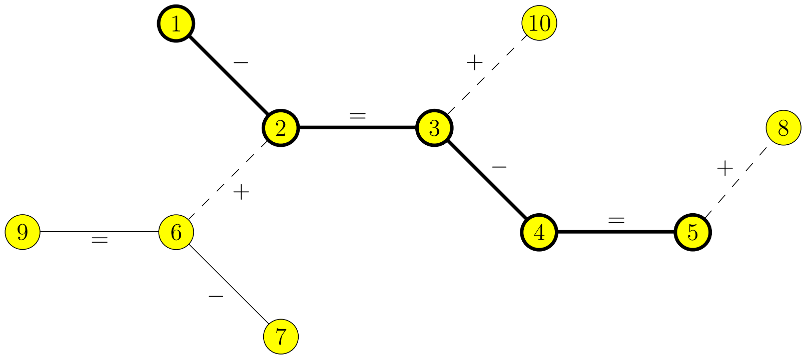

Fig. 11. Step 1: Prune auxiliary branches to isolate B.

- if $a \in B$, $b \in B$, B is a positive chain, and $a \hat{=} b$ in G, then $a \hat{+} b$ in $J_B(G)$,
- if $a \in B$, $b \in B$, B is a negative chain, and $a \hat{=} b$ in G, then $a \hat{-} b$ in $J_B(G)$,
- if $a \notin B$ or $b \notin B$, and $a\hat{R}b$ in G, then $a\hat{R}b$ in $J_B(G)$, for $R \in \{+, =, -\}$.

It is readily verified that $J_B(G)$ is a tree of relations. We note that $B' = J_B(B)$ is again a signed chain in $J_B(G)$. The mapping $(G, B) \mapsto J_B(G)$ may be described geometrically in three simple steps as shown in Figs. 11–13: we consider the tree of relations in Fig. 1 and the highlighted negative chain B consisting of vertices $\{1, 2, 3, 4, 5\}$ (see Fig. 10). The resulting tree is shown in Fig. 14.

The induction on a disjoint union of signed chains, though it is not effectively used in the present paper, is an important tool in the definition of the induction on interval exchange transformations (Section 3 below):

Definition 3.5. For a union $B = B_1 \cdots \cup B_k$ of piecewise disjoint signed chains, we define $J_B(G)$ as the composition $J_{B_k} \circ \cdots J_{B_1}(G)$, which by Definition 3.4 above is independent of the order of the B_i.

Example 3.6. We look again at the trees in Section 2 above.

Let G be $1\hat{-}3\hat{+}2$. Then $s = (123)$, $t = (132)$, $u = (321)$. The positive chains are $B_1 = 3\hat{+}2$, $B_2 = 1$; the negative chains are $B_3 = 1\hat{-}3$ and $B_4 = 2$. $J_{B_1}(G)$ is $1\hat{-}3\hat{=}2$, $J_{B_3}(G)$ is $1\hat{=}3\hat{+}2$, and $J_{B_2}(G)$ and $J_{B_4}(G)$ are G. When we went from state 0 to 1, we induced successively on the two negative chains B_3 and B_4, and thus by Definition 3.5 on the union $B_3 \cup B_4$.

Let G be $1\hat{=}3\hat{+}2$. Then $s = (321)$, $t = (132)$, $u = (123)$. The only positive chain is $B_1 = 1\hat{=}3\hat{+}2$; the negative chains are $B_2 = 1\hat{=}3$ and $B_3 = 2$. $J_{B_1}(G)$ is $2\hat{=}1\hat{+}3$, $J_{B_2}(G)$ is $1\hat{-}3\hat{+}2$, and $J_{B_3}(G)$ is G. When

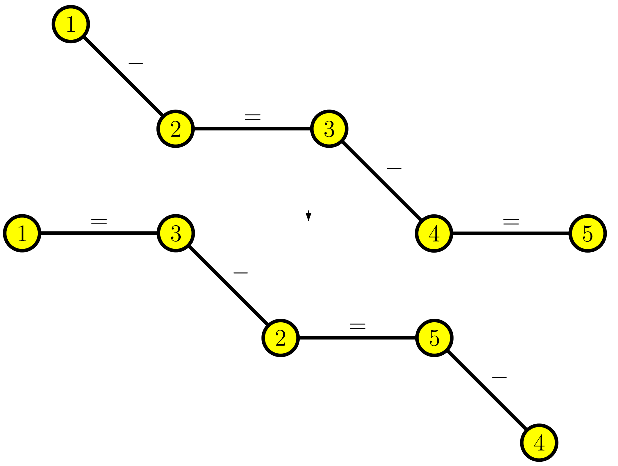

Fig. 12. Step 2: Exchange vertices $a \leftrightarrow s(a)$ and edges $- \leftrightarrow =$.

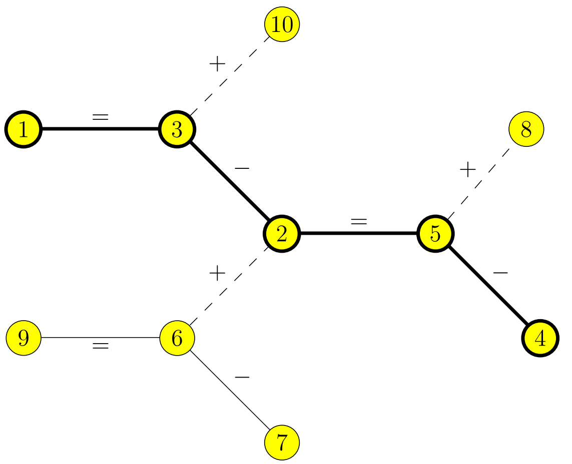

Fig. 13. Step 3: Re-join pruned branches to their original connections.

we went from state 1 to 2, we induced on the negative chain B_3, and from state 2 to state 3 we induced on the positive chain B_1.

Let G be $2\hat{=}1\hat{+}3$; to go from state 3 to 4, we induced on the union of the two negative chains $2\hat{=}1$and 3.

We can now give the full rules of the self-dual induction in [3]. At a given stage, they depend both on the relations between l_i and r_i, coded by a tree of relations G with first bijection s, and on the signs of the $l_i - r_{s(i)} = l_{s(i)} - r_i$. Namely, let B be the union of all positive chains on which $l_i > r_{s(i)}$ on every vertex, and of all negative chains on which $l_i < r_{s(i)}$ on every vertex; then, if i is a vertex of a positive chain in B, E_i is cut on the left by an amount $r_{s(i)}$, while if i is a vertex of a negative chain in B, E_i is cut on the right by an amount $l_{s(i)}$; if i is a vertex outside of B, E_i is not cut. It is proved in [3] that *the tree of relations at the next stage is* $J_B(G)$. Note that the two other bijections of the tree G are also used in [3], but for technical reasons there we use slightly different maps, namely $p = ts$ and $m = us$.

As is explained in [3], these rules, and the definitions of trees and induction, come naturally from the requirements of the self-dual induction, and this theory needs the whole machinery of trees of relations to work satisfactorily.

The proof of the following lemma is immediate from the above definitions:

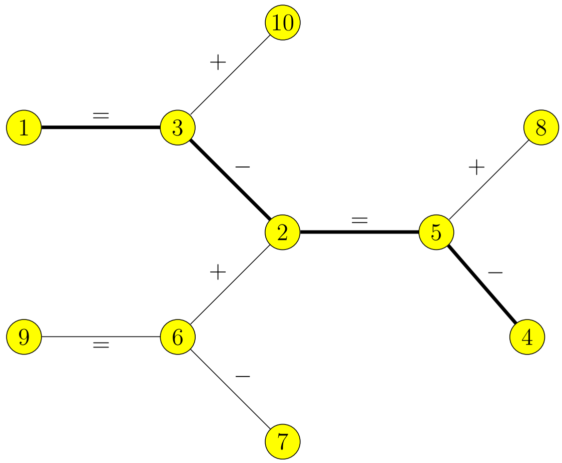

Fig. 14. The resulting tree of relations.

Lemma 3.7. *Let B a signed chain of a tree of relations G. The bijections (s', t', u') of $J_B(G)$ are given as follows:*

- *if $a \in B$ and B is a positive chain, $s'(a) = sts(a)$, $t'(a) = s(a)$, $u'(a) = u(a)$;*
- *if $a \in B$ and B is a negative chain, $s'(a) = sus(a)$, $t'(a) = t(a)$, $u'(a) = s(a)$;*
- *if $a \notin B$, $s'(a) = s(a)$, $t'(a) = t(a)$, $u'(a) = u(a)$.*

4. Graphs of graphs

In this section we use the induction mapping to construct a graph whose vertices consist of trees of relations with k vertices, and where the directed edges between vertices are defined in terms of the induction mapping.

Definition 4.1. For a given tree of relations G, let $\Gamma(G)$ be the smallest set of trees of relations on K which contains G and is closed under induction.

We give $\Gamma(G)$ the structure of an oriented graph as follows: for each $G' \in \Gamma(G)$ and each signed edge B of G', we place a directed edge from G' to $J_B(G')$ labeled $+$ (resp. $-$) if B is a positive (resp. negative) chain. We call $\Gamma(G)$ a *graph of graphs*.

Let k be a positive integer. We define the *initial tree of relations* on the set $K = \{1, 2, \ldots, k\}$, denoted as $G_0(k)$, by

$$G_0(k) = 1 \hat{-} k \hat{+} 2 \hat{-} (k-1) \hat{+} 3 \hat{-} (k-2) \ldots .$$

As we saw in Section 2 for $k = 3$, this is the tree of relations which codes the relations between the parameters of the self-dual induction in the initial state for an interval exchange transformation on $k+1$ intervals, with suitable conditions on the permutation which rearranges the intervals, and on the positions of the discontinuities.

We denote by $\Gamma(k)$ the graph of graphs $\Gamma(G_0(k))$. Figs. 15–17 illustrate $\Gamma(1)$, $\Gamma(2)$ and $\Gamma(3)$ (the highlighted edges in $\Gamma(3)$ correspond to the example in Section 2). We shall see later that $\Gamma(4)$ has 28 vertices while $\Gamma(5)$ has 90 vertices.

5. Shapes and fillings

In the next three sections we shall investigate the structure of $\Gamma(k)$, and in particular determine its cardinality. We begin by introducing the following two auxiliary notions.

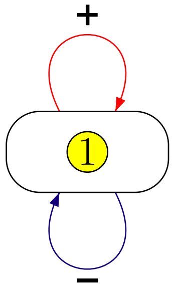

Fig. 15. The graph of graphs $\Gamma(1)$.

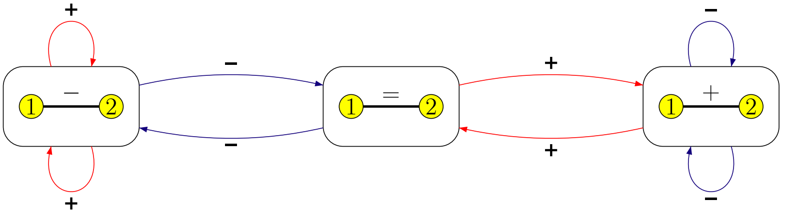

Fig. 16. The graph of graphs $\Gamma(2)$.

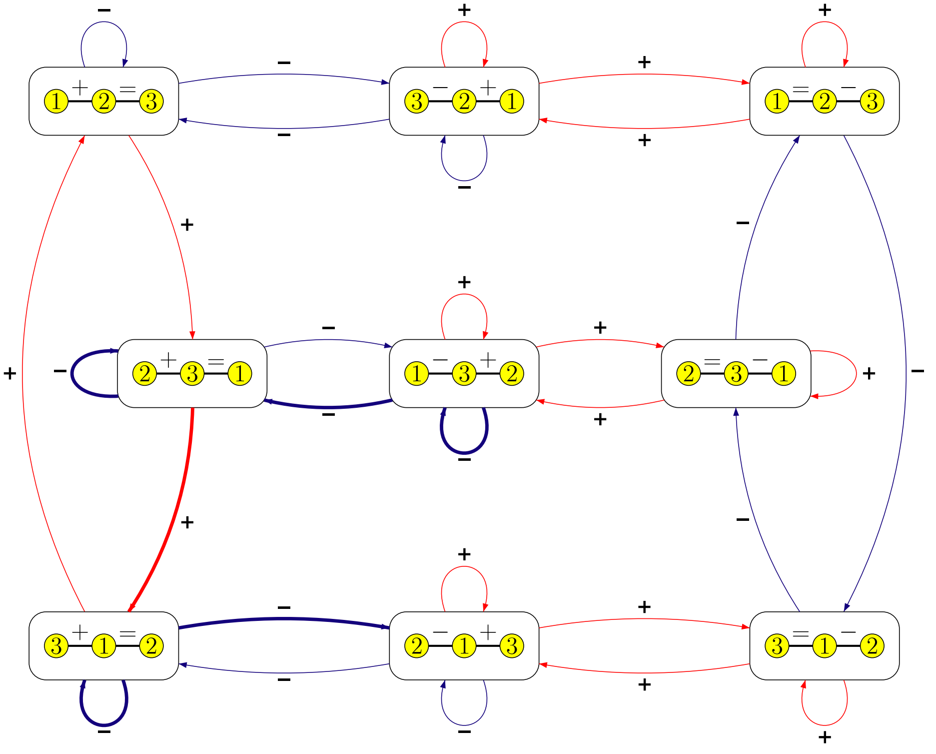

Fig. 17. The graph of graphs $\Gamma(3)$.

Definition 5.1. A *shape* is a (non-oriented) tree F with k unnamed vertices and $k-1$ edges labeled $+$, $-$, or $=$, such that two adjacent edges never have the same label.

The *shape of a tree of relations* G is the tree obtained from G by removing the labels of the vertices. We say that G is a *filling* of its shape.

A *rooted* tree of relations (resp. shape) is a tree of relation (resp. shape) together with the choice of one vertex, called the *root*.

Proposition 5.2. *For any tree of relations G, there exists a tree of relations $G_\star$ without any $=$ edge and a sequence of inductions $J_{B_1}, \dots, J_{B_n}$ such that $G_\star = J_{B_n} \cdots J_{B_1}(G)$.*

Proof. If G has no $=$ edge, we are done; otherwise, we shall relate, by a sequence of inductions, G to a tree of relations G' having one less $=$ edge.

An $=$ edge between two vertices a and b has at most four adjacent edges $a \hat{-} y_1, a \hat{+} y_2, b \hat{-} y_3, b \hat{+} y_4$; for $y \in \{y_1, \dots, y_4\}$ let $G_y(a, b)$ be the connected component containing y of the tree G deprived of the edge from y to its adjacent a or b vertex. We say that $a \hat{=} b$ is an *extremal* $=$ edge if there is at most one i such that $G_{y_i}(a, b)$ has at least one $=$ edge; if it exists, we call this $G_{y_i}(a, b)$ the *dangerous* subtree of $a \hat{=} b$; note that the non-dangerous $G_{y_i}(a, b)$ contain no vertex with more than two adjacent edges, because three edges adjacent to one common vertex must have three different labels. For example, the $=$ edges between vertices 9 and 6 and between vertices 4 and 5 in Fig. 1 are extremal, while the $=$ edge between vertices 2 and 3 is not extremal.

There is at least one extremal $=$ edge, since otherwise we can follow a directed infinite path in G and G is not a finite tree.

Suppose $a \hat{=} b$ is an extremal edge of $G = G_0$, and suppose first that it has a dangerous subtree and the edge leading to it is a $+$ edge. We denote by b_0 the vertex which is on that edge and on the extremal edge, and by a_0 the other vertex on the extremal edge.

We build a finite sequence of graphs G_n such that

- G_{n+1} is obtained from G_n by a sequence of one or two inductions of sign $(-1)^{n+1}$;
- if n is even, G_n has an extremal $=$ edge $a_n \hat{=} b_n$, with at most four adjacent edges $a_n \hat{-} x_n$, $a_n \hat{+} y_n$, $b_n \hat{-} z_n$, $b_n \hat{+} t_n$, such that t_n exists, $G_{t_n}(a_n, b_n)$ is made of the union of $G_{t_0}(a_0, b_0)$ and a branch from t_0 to t_n with n vertices (t_0 excluded, t_n included), and is the dangerous subtree of $a_n \hat{=} b_n$;
- if n is odd, the same is true with all signs changed to the opposite.

This is true for $n = 0$, for a unique choice of (x_0, y_0, z_0, t_0). Suppose n is even; then we consider the four possibilities for the negative chain containing the edge $a_n \hat{=} b_n$:

- if it is $x_n \hat{-} a_n \hat{=} b_n \hat{-} z_n$, we induce on it, getting the negative chain $z_n \hat{=} a_n \hat{-} b_n \hat{=} x_n$, and induce on this new chain, getting G_{n+1} with the negative chain $a_n \hat{-} z_n \hat{=} x_n \hat{-} b_n$. Then we put $a_{n+1} = y_n$, $b_{n+1} = x_n$.
- If it is $x_n \hat{-} a_n \hat{=} b_n$, we induce on it, getting the negative chain $x_n \hat{=} b_n \hat{-} a_n$, and induce on this new chain, getting G_{n+1} with the negative chain $b_n \hat{-} x_n \hat{=} a_n$. Then we put $a_{n+1} = a_n$, $b_{n+1} = x_n$.
- If it is $a_n \hat{=} b_n \hat{-} z_n$, we induce on it, getting G_{n+1} with the negative chain $b_n \hat{-} a_n \hat{=} z_n$. Then we put $a_{n+1} = z_n$, $b_{n+1} = b_n$.
- If it is $a_n \hat{=} b_n$, we induce on it, getting G_{n+1} with the negative chain $b_n \hat{-} a_n$ and we stop the process.

For n odd we do the same construction, changing each sign to its opposite; and the sequence G_n has the claimed properties; note that G_{n+1} has the same number of $=$ edges as G_n, except at the last step where this number decreases by 1. If the dangerous subtree of $a \hat{=} b$ in G_0 is linked to b_0 by a $-$ edge, we do the same process with all signs changed. If there is no dangerous subtree of $a \hat{=} b$ in G_0, but G_0 is not reduced to $a \hat{=} b$, we choose b_0 to be a or b, and t_0 such that $b_0 \hat{e_0} t_0$, where $e_0 = +$ or $e_0 = -$ and do the same construction as above, defining t_n by $b_n \hat{e_n} t_n$ where e_n is the sign of $(-1)^n e_0$; all of our assertions remain true except that $G_{t_n}(a_n, b_n)$ is not the dangerous subtree of $a_n \hat{=} b_n$. If G_0 is reduced to $a \hat{=} b$, we define G_1 as the tree $a \hat{-} b$ and stop the process. In all cases, as all the G_n have the same finite number of vertices, the process has to stop, and the final $G_n = G'$ has one $=$ edge less than G_0. $\square$

Corollary 5.3. *If G has k vertices, every possible shape with k vertices appears as the shape of a tree of relations in $\Gamma(G)$.*

Proof. By Proposition 5.2, it is enough to show that every shape without $=$ edges appears. If k is odd, there is only one such shape; the shape of the initial tree $\hat{-}.\hat{+}\cdots\hat{+}$ and the result is proved.

If k is even, the shapes without $=$ edges are $\hat{-}.\hat{+}\cdots\hat{-}$ and $\hat{+}.\hat{-}\cdots\hat{+}$; we have shown that $\Gamma(G)$ contains one tree with one of these shapes, for example $a_1\hat{-}a_2\hat{+}a_3\cdots a_{2p-1}\hat{-}a_{2p}$; then by a negative induction $\Gamma(G)$ contains also $a_1\hat{=}a_2\hat{+}a_3\hat{=}\cdots a_{2p-1}\hat{=}a_{2p}$, hence by a positive induction $a_2\hat{+}a_1\hat{=}a_4\hat{+}a_3\cdots\hat{=}a_{2p}\hat{+}a_{2p-1}$, and hence by a negative induction $a_2\hat{+}a_1\ \hat{-}a_4\hat{+}a_3\cdots\hat{-}a_{2p}\hat{+}a_{2p-1}$; thus the other one of the two shapes is the shape of at least one tree in $\Gamma(G)$, and similarly if we start from the opposite one. $\square$

6. Circular order, and description of the graph of graphs

Lemma 6.1. *Let G be a tree of relations, and s, t, u its bijections; we say that b is the successor of a if $b = tsu(a)$; this defines a total circular order on the vertices of G, invariant by any induction.*

Proof. We check first the invariance under the induction J_B for B a signed chain. Let s', t', u' be as in Lemma 3.7; suppose that $a \in B$ and B is a negative chain; then $u'a = sa$ is in B, $s'u'a = sussa = sua$ is in B, and thus $t's'u'a = t'sua = tsua$; similarly, if $a \in B$ and B is a positive chain, we get $t's'u'a = sstsua = tsua$; if a is not in B $t's'u'a = tsua$.

Because of this invariance and Proposition 5.2, we need only check that we have a total circular order for trees without $=$ edges. And for a tree $a_1\hat{-}a_2\hat{+}a_3\cdots\hat{-}a_{2p}$ we get the order $(a_1, a_3, \ldots, a_{2p-1}, a_{2p}, a_{2p-2}, \ldots, a_2, a_1)$; for a tree $a_1\hat{+}a_2\hat{-}a_3\cdots\hat{+}a_{2p}$ we get the order $(a_1, a_2, \ldots, a_{2p-2}, a_{2p}, a_{2p-1}, \ldots, a_3, a_1)$; for a tree $a_1\hat{-}a_2\hat{+}a_3\cdots\hat{+}a_{2p+1}$ we get the order $(a_1, a_3, \ldots, a_{2p+1}, a_{2p}, a_{2p-2}, \ldots, a_2, a_1)$. $\square$

The circular order described above may be described geometrically as follows: starting from any vertex x in a tree of relations G, we move from x to the vertex y where x and y are joined by a $-$ edge. If x is not incident to a $-$ edge, we take y to be x. Next we move from y to z where y and z are joined by an $=$ edge. Again, if no such edge exists, we take z to be y. Finally we move from z to w where w is joined to z by a $+$ edge. Then w is the successor of x. For the tree in Fig. 1, the circular order is $(1, 10, 3, 8, 5, 4, 6, 7, 9, 2, 1)$ while for every tree in Example 3.5 it is $(1, 2, 3, 1)$.

Proposition 6.2. *A tree of relations G is in $\Gamma(G')$ if and only if the circular order of its vertices, given by t, is the same as that of G'.*

Proof. By Lemma 6.1, the condition is necessary. By Proposition 5.2, it is enough to check the sufficiency for trees of relations without $=$ edges.

If k is odd, the only shape is $\hat{-}.\hat{+}\cdots\hat{+}$; for it, every possible filling is of the form $a_1\hat{-}a_2\hat{+}a_3\cdots\hat{+}a_{2p+1}$ where the circular order $(a_1, a_3, \ldots, a_{2p+1}, a_{2p}, a_{2p-2}, \ldots, a_2, a_1)$ coincides with the circular order on G' by assumption. This makes k trees of relations, one of which belongs to $\Gamma(G')$ by Corollary 5.3. We call it $a_1^1\hat{-}a_2^1\hat{+}a_3^1\hat{-}\cdots\hat{+}a_{2p+1}^1$; all the others can be reached from it by induction, first by negative inductions going to $a_1^1\hat{=}a_2^1\hat{+}a_3^1\hat{=}\cdots\hat{+}a_{2p+1}^1$, then by inducing successively $1 \le l \le k$ times on the whole positive chain and ending with negative inductions to replace $=$ edges by $-$ edges.

If k is even, take the shape $\hat{-}.\hat{+}\cdots\hat{-}$; for it, every possible filling is of the form $a_1\hat{-}a_2\hat{+}a_3\cdots\hat{-}a_{2p}$ where the circular order $(a_1, a_3, \ldots, a_{2p-1}, a_{2p}, a_{2p-2}, \ldots, a_2, a_1)$ coincides with the order of G'. This gives $\frac{k}{2}$ trees of relations. One of them belongs to $\Gamma(G')$ by Corollary 5.3, and we call it $a_1^1\hat{-}a_2^1\ \hat{+}a_3^1\cdots\hat{-}a_{2p-1}^1$; all the others can be reached from it, first by negative inductions going to $a_1^1\hat{=}a_2^1\hat{+}\ a_3^1\hat{=}\cdots\hat{+}a_{2p-1}^1$, then inducing successively $2 \le 2l \le 2k$ times on the whole positive chain, and ending with negative inductions. The proof is similar for the shape $\hat{+}.\hat{-}\cdots\hat{+}$. $\square$

Corollary 6.3. *If G is a tree of relations with k vertices, then $\Gamma(G)$ is obtained from $\Gamma(k)$ by a renumbering of the vertices. G is in $\Gamma(k)$ if and only if its circular order is $(1, 2, \ldots, k, 1)$.*

Proof. Immediate from Proposition 6.2 and computation of the circular order of $G_0(k)$. $\square$

7. Cardinality of the graph of graphs

Lemma 7.1. *Let F be a shape, and σ a bijection (vertex to vertex, edge to edge, preserving the labels) such that $\sigma F = F$. Then σ is an involution; if σ is not the identity, k is even and F is the disjoint union of two subtrees F_1 and F_2, and an edge e such that $\sigma e = e$, $\sigma F_1 = F_2$, $\sigma F_2 = F_1$.*

For a given F there is at most one such σ different from the identity.

Proof. We consider σ as an isometry of a compact metric space by replacing edges by segments of length 1. Thus, σ has a fixed point.

If the fixed point is a vertex, σ has to fix the adjacent edges (which are all distinct) and hence the adjacent vertices and, continuing this reasoning, we get that σ is the identity.

If the fixed point is an edge e, either σ fixes its two end vertices or it exchanges them. In the first case, again σ is the identity. In the second case, we get the desired decomposition given above and thus k is even. And σ^2 fixes F_1 and one of its vertices; thus it is the identity on F_1 and similarly on F_2, and thus on F.

For a given F, if it exists e is unique (as there is the same number of vertices on each side) and σ is defined uniquely on the adjacent edges and thus everywhere. □

Definition 7.2. A shape F is said to be *symmetric* if there exists a σ as in Lemma 7.1, different from the identity. We call such a σ a *symmetry*.

Lemma 7.3. *If k is odd, every shape has k different fillings in $\Gamma(k)$; if k is even, every symmetric shape has $\frac{k}{2}$ different fillings and every non-symmetric shape has k different fillings.*

Proof. Given a shape F, we fix a way to relate it by a sequence of inductions, as in the proof of Proposition 5.2, to a shape F' without $=$ edges; if F is non-symmetric, this defines a map ϕ from the fillings G of F to the fillings G' of F' (if ϕ gives a different image to one filling written in two different ways, this defines a symmetry on F).

If F and F' are non-symmetric, then ϕ is a bijection. This happens if k is odd by Lemma 7.1 and in this case we need only consider the shape $F' = \hat{-}.\hat{+}\cdots\hat{+}$; we have seen in the proof of Proposition 6.2 that it has k fillings, and thus so has F.

If k is even and F is non-symmetric; then F' is one of the (symmetric) shapes $\hat{-}.\hat{+}\cdots\hat{-}$ and $\hat{+}.\hat{-}\cdots\hat{+}$, each of which has $\frac{k}{2}$ fillings and ϕ is two-to-one; hence F has k fillings.

If k is even and F is symmetric, then we can relate F to an F' without $=$ edges such that at each stage the shape is symmetric (by working simultaneously on one extremal $\hat{=}$ in F_1 and its image under the symmetry); thus our ϕ sends the symmetry of F to the (unique) symmetry of F', and thus ϕ is well defined and one-to-one, and hence F has $\frac{k}{2}$ fillings. □

Corollary 7.4. *$\Gamma(k)$ contains k trees of relations without $=$ edges.*

Proposition 7.5.

$$\#\Gamma(k) = Cat_{k+1} - Cat_k$$

where $Cat_k = \frac{(2k)!}{(k+1)(k!)^2}$ is the kth Catalan number.

The number of different shapes is $\frac{Cat_{k+1}-Cat_k}{k}$ if k is odd and $\frac{Cat_{k+1}-Cat_k}{k} + \frac{3}{2}Cat_{\frac{k}{2}}$ if k is even.

Proof. We count first the number $\rho(k)$ of rooted shapes (where we have specified one vertex; see Definition 5.1 above) on k letters. We define four quantities:

- $\rho_0(k)$ is the number of rooted shapes with no edge from the root;
- $\rho_1(k)$ is the number of rooted shapes with one edge from the root, labeled $+$ (resp. $=$, resp. $-$), these three numbers being equal;
- $\rho_2(k)$ is the number of rooted shapes with two edges from the root, labeled $+$ and $-$ (resp. $=$ and $-$, resp. $+$ and $=$);

- $\rho_3(k)$ is the number of rooted shapes with three edges from the root;
- $\zeta(k)$ is the number of rooted shapes with no edge from the root labeled $+$ (resp. $=$, resp. $-$).

We have:

- $\rho(k) = \rho_0(k) + 3\rho_1(k) + 3\rho_2(k) + \rho_3(k)$;
- $\zeta(k) = \rho_0(k) + 2\rho_1(k) + \rho_2(k)$;
- $\rho_0(1) = 1$, $\rho_0(k) = 0$ if $k > 1$;
- $\rho_1(k) = \zeta(k-1)$;
- $\rho_2(k) = \sum_{p+q=k-1} \zeta(p)\zeta(q)$;
- $\rho_3(k) = \sum_{p+q+r=k-1} \zeta(p)\zeta(q)\zeta(r)$.

In terms of the power series $R_i = \sum_{k\geq 1} \rho_i(k)X^k$, $Z = \sum_{k\geq 1} \zeta(k)X^k$ we get $R_1 = XZ$, $R_2 = XZ^2$, $R_3 = XZ^3$. Hence $Z = X(Z^2 + 2Z + 1)$, $XZ^2 + (2X-1)Z + X = 0$, and the only admissible solution is $Z = \frac{1-\sqrt{1-4X}}{2X} - 1$. This gives $\zeta(k) = \mathrm{Cat}_k$.

Now $R = X(Z+1)^3 = Z(Z+1) = \frac{Z}{X} - Z - 1$; thus $\rho(k) = \zeta(k+1) - \zeta(k)$.

If k is odd, one shape gives k rooted shapes, so the number of shapes is $\frac{\rho(k)}{k}$ and the number of trees of relations in Γ_k is $\rho(k)$ by Lemma 7.3.

If k is even, a symmetric shape is made with one central edge (three choices) and a compatible rooted shape on $\frac{k}{2}$ letters; thus the number $\tau(k)$ of symmetric shapes is $3\zeta(\frac{k}{2})$. A symmetric shape corresponds to $\frac{k}{2}$ rooted shapes and a non-symmetric shape corresponds to k rooted shapes; if $\psi(k)$ is the number of non-symmetric shapes, $\rho(k) = \frac{k}{2}\tau(k) + k\psi(k)$. By Lemma 7.3 the number of trees of relations in Γ_k is thus $\rho(k)$ and, by computing $\psi(k)$, we get the claimed number of shapes. $\square$

Note that if we fix an order on the labels, such as $-$ smaller than $=$ and $=$ smaller than $+$, the rooted shapes whose roots have no $-$ (resp. $=$, $+$) edge, whose number is $\zeta(k)$, are in bijection with the set of ordered (incomplete) binary trees (suspending them by the root) and this proves again that $\zeta(k)$ is the kth Catalan number; see [8] for example.

The sequence of numbers of shapes begins with $1, 3, 3, 10, 18, 57\ldots$ and seems to be a new sequence, not yet in the *On-line Encyclopedia of Integer Sequences* [6].

The third author, together with Marsh and Schroll, has shown that the set of shapes on k vertices is in bijection with the set of all labeled triangulations of a regular $(k+2)$-sided polygon up to rotations, where the edges of each triangle are labeled $+$ ($=$, $-$) in the clockwise direction. Although we do not exploit this point in this paper, the induction mapping may be defined on shapes by simply forgetting the labeling of the vertices. In this way, the induction mapping may be regarded as a mapping defined on labeled triangulated polygons. This alternative perspective leads to another proof of the results obtained in Section 7 by way of a formula due to Brown [1] for the number of triangulations of a regular $(k+2)$-sided polygon up to rotations, which incidentally corresponds to the number of isomorphism classes of (basic) cluster-tilted algebras of type A_{k-1} [7].

8. Secondary structures of genetic sequences

In Section 6 we associated a circular order with a tree structure; now we start from a circular order and a structure imitated from the secondary structures of RNA (see for example [2]) and get trees of relations. Namely:

Definition 8.1. Let S be the periodic circular string on three symbols $(XYZ)^k$; we equip it with an origin and denote it by $X_1Y_1Z_1 \cdots X_kY_kZ_k$. A pseudo-knot-free secondary structure Σ on S is a set of links between two different instances of symbol X, or two different instances of symbol Y, or two different instances of symbol Z, such that any pair of distinct links, drawn inside the circle, have an empty intersection.

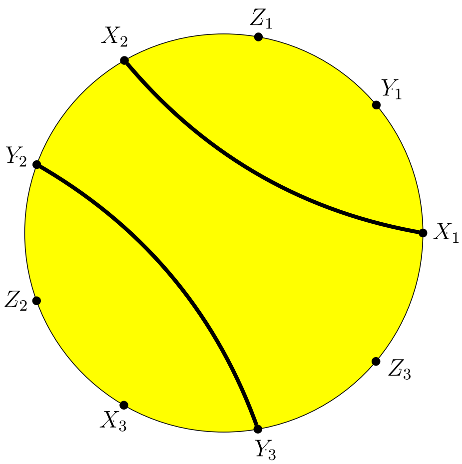

Fig. 18. $1 \hat{+} 2 \hat{=} 3$.

Proposition 8.2. *Let Σ be a pseudo-knot-free secondary structure as above. We define a graph G by putting $a \hat{+} b$ (resp. $a \hat{=} b$, resp. $a \hat{-} b$) if there is a link between X_a and X_b (resp. Y_a and Y_b, resp. Z_a and Z_b). Then G is a disjoint union of trees of relations G_i, $1 \le i \le d$, such that if $i \ne j$, a_1 and a_2 are vertices of G_i and b_1 and b_2 are vertices of G_j, we cannot have $a_1 < b_1 < a_2 < b_2$ in the circular order $(1, \dots, k, 1)$. We can then define the maps s, t, u as in Section 3. For any vertex a of G_i, $tsu(a)$ is the next element of G_i in the circular order $(1, \dots, k, 1)$.*

Proof. Note first that two adjacent edges in G have different labels; otherwise two different links in Σ have a nonempty intersection.

We show that G has no loop. Suppose that there is a loop with vertices $a_1, \dots, a_r$; then it cannot be the case that all of its edges are labeled $=$. If there is an edge $a_i \hat{+} b_i$, there is a link between X_{a_i} and X_{b_i}. Then any link from Y_{a_i} or Z_{a_i} not intersecting this X-link goes to Y_c or Z_c for some $a_i < c < b_i$ (in the circular order), while any link from Y_{b_i} or Z_{b_i} not intersecting the X-link goes to Y_d or Z_d for some $b_i < d < a_i$ (in the circular order), and there is no way to close the loop. A similar reasoning applies if there is an edge $a_i \hat{-} b_i$.

Thus G is indeed a disjoint union of trees of relations G_i and the condition on four vertices is necessary to avoid nonempty intersections. For a vertex a of G_i, either $u(a) = a$ or there is a link between Z_a and $Z_{u(a)}$, either $su(a) = u(a)$ or there is a link between $Y_{su(a)}$ and $Y_{u(a)}$, and either $tsu(a) = su(a)$ or there is a link between $Z_{su(a)}$ and $Z_{tsu(a)}$. Thus $tsu(a)$ is a vertex of G_i and, to avoid nonempty intersections, every vertex situated strictly between a and $tsu(a)$ can be linked only to another vertex strictly between a and $tsu(a)$; thus such a vertex is not in G_i. $\square$

Proposition 8.3. *Let G be a disjoint union of trees of relations G_i, $1 \le i \le d$; we equip the set of all vertices of the G_i with any circular order compatible with the circular order tsu defined on each G_i and such that if a_1 and a_2 are vertices of G_i, and b_1 and b_2 are vertices of G_j, we do not have $a_1 < b_1 < a_2 < b_2$ in this order. We define a link between X_a and X_b (resp. Y_a and Y_b, resp. Z_a and Z_b) whenever there is an edge $a \hat{+} b$ (resp. $a \hat{=} b$, resp. $a \hat{-} b$) in G; then we get a pseudo-knot-free secondary structure as above.*

Proof. What we have to prove is that any two distinct links have a nonempty intersection. When we have one tree of relations G, this is trivially true if G has no $=$ edge; and the definition of the induction in Section 3 implies that this property is stable under induction. Thus the result follows by Proposition 5.2. When we have several trees, the condition on the order allows us to mix the structures without creating intersections. $\square$

Proposition 8.4. *A single tree of relations defines a pseudo-knot-free secondary structure which is maximal: no link can be added on the same set of vertices.*

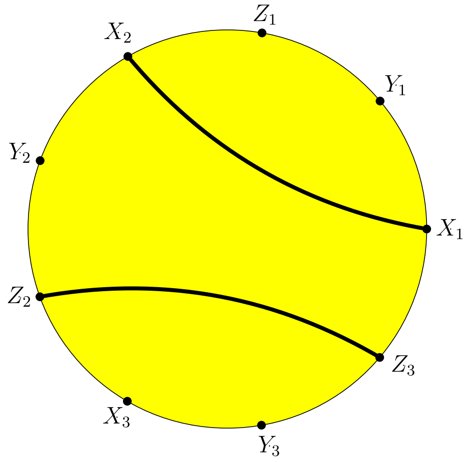

Fig. 19. $1\hat{+}2\hat{-}3$.

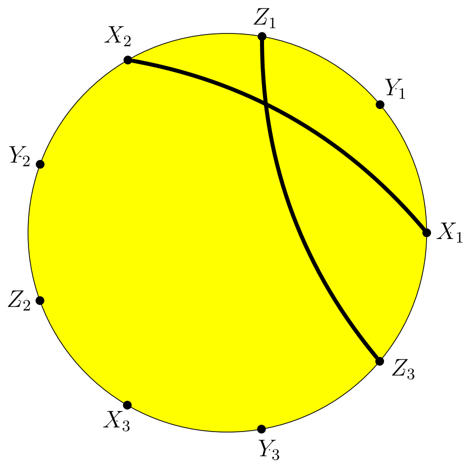

Fig. 20. $3\hat{-}1\hat{+}2$.

Proof. Any extra link would add an extra edge, but by Proposition 8.2 the new graph has to be a union of trees. □

Figs. 18 and 19 illustrate pseudo-knot-free structures corresponding to the trees of relations $1\hat{+}2\hat{=}3$ and $1\hat{+}2\hat{-}3$ in $\Gamma(3)$. Fig. 20 illustrates an intersection between the arcs for the tree of relations $3\hat{-}1\hat{+}2$ not contained in $\Gamma(3)$ (of course there would be no intersection if we used the circular order defined by $3\hat{-}1\hat{+}2$, namely $(1, 3, 2, 1)$).

Example 8.5. The forest $1\hat{+}2\hat{-}3$, $4\hat{=}5$ also defines a maximal pseudo-knot-free secondary structure.

Thus, to ensure that a given structure Σ on $(XYZ)^k$ corresponds to a single tree of relations, we need to specify that Σ has $k-1$ links.

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